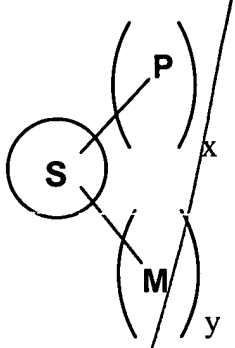
## *Claims*

We claim:

1.A polypharmacophore comprising the general formula (I):




(I)

wherein **S** comprises a scaffold unit; **P** comprises a pharmacophore unit, wherein x is greater than or equal to two; and **M** comprises a modifier unit, wherein y is greater than or equal to 0, whereby each one of **P** and **M**, for each occurrence, is appended to said scaffold unit, and whereby the polypharmacophore interacts with at least two biological targets.

2. The polypharmacophore of claim 1, wherein said scaffold unit is synthesized using a domino reaction.

3. The polypharmacophore of claim 1, wherein said polypharmacophore is used to treat, prevent, mitigate or slow progression of a condition or disease implicating biological systems which act in concert.

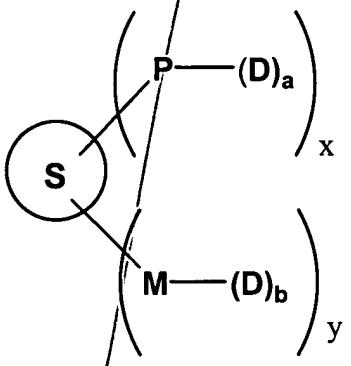
4. The polypharmacophore of claim 1, wherein said polypharmacopore is used to modulate the function of the dopaminergic system.

5. The polypharmacophore of claim 1, wherein said polypharmacophore is used to treat diseases and conditions selected from the group consisting of Alzheimer's Disease, Huntington's Disease, depression, attention deficit disorder, ADHD, autism, obesity and inflammation.

6. The polypharmacophore of claim 1, wherein said pharmacophoric units are selected from the group consisting of D-1 agonist, D-2 agonist, D-3 agonist, D-4 agonist, irreversible monoamine inhibitor, reversible monoamine inhibitor, monoamine transporter inhibitor, COMT inhibitor, MAO inhibitor and dopamine transporter inhibitor.

7. The polypharmacophore of claim 1, wherein said modifier unit is selected from the group of spacer, scaffold assembler, delivery modulator, bioactivating group, detection agent, agent to increase solubility, and targeting agent.

8. A polypharmacophore comprising the general formula **(IA)**:




**(IA)**

wherein **S** comprises a scaffold unit; **P** comprises a pharmacophore unit, wherein x is greater than or equal to 2; **M** comprises a modifier unit, wherein y is greater than or equal to 0, whereby each one of **P** and **M**, for each occurrence, is appended to said scaffold unit; and **D** comprises an additional modifier unit, wherein a and b, for each occurrence of x or y, are each independently greater than or equal to zero, and wherein **D** may also be directly attached to one or more

pharmacophores **(P)** and alternatively or additionally to one or more existing modifier units **(M)** that are attached to the scaffold, and whereby the polypharmacophore interacts with at least two biological targets.

9. The polypharmacophore of claim 8, wherein said scaffold unit is synthesized using a domino reaction.

10. The polypharmacophore of claim 8, wherein said polypharmacophore is used to treat and/or prevent a condition or disease implicating biological sites which act in concert.

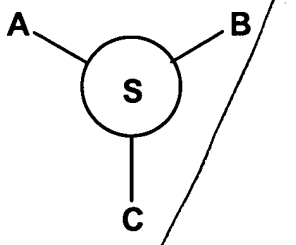
11. The polypharmacophore of claim 8, wherein said polypharmacopore is used to modulate the function of the dopaminergic system.

12. The polypharmacophore of claim 8, wherein said polypharmacophore is used to treat diseases and conditions selected from the group consisting of Alzheimer's Disease, Huntington's Disease, depression, attention deficit disorder, autism, obesity and inflammation.

13. The polypharmacophore of claim 8, wherein said pharmacophoric units are selected from the group consisting of D-1 agonist, D-2 agonist, D-3 agonist, D-4 agonist, irreversible monoamine inhibitor, reversible monoamine inhibitor, monoamine transporter inhibitor, COMT inhibitor, MAO inhibitor and dopamine transporter inhibitor.

14. The polypharmacophore of claim 8, wherein said modifier unit is selected from the group of spacer, scaffold assembler, delivery modulator, bioactivating group, detection agent, agent to increase solubility, and targeting agent.

15. A polypharmacophore comprising the general formula **(II):**




(II)

wherein S comprises a scaffold unit; at least two of A, B, or C comprise a pharmacophore; and wherein one or none of A, B, or C comprise a modifier unit, whereby the polypharmacophore interacts with at least two biological targets.

16. The polypharmacophore of claim 15, wherein said scaffold unit is synthesized using a domino reaction.

17. The polypharmacophore of claim 15, wherein said polypharmacophore is used to treat and/or prevent a condition or disease implicating biological systems which act in concert.

18. The polypharmacophore of claim 15, wherein said polypharmacopore is used to modulate the function of the dopaminergic system.

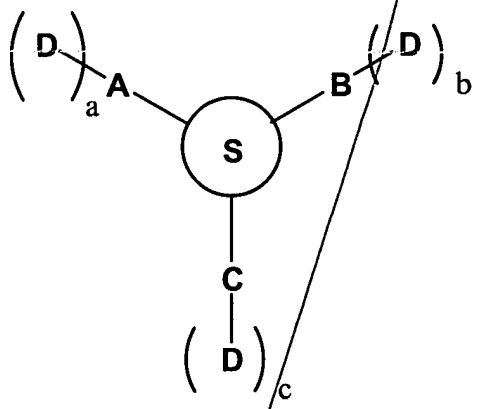
19. The polypharmacophore of claim 15, wherein said polypharmacophore is used to treat diseases and conditions selected from the group consisting of Alzheimer's Disease, Huntington's Disease, depression, attention deficit disorder, autism, obesity and inflammation.

20. The polypharmacophore of claim 15, wherein said pharmacophoric units are selected from the group consisting of D-1 agonist, D-2 agonist, D-3 agonist, D-4 agonist, irreversible monoamine inhibitor, reversible monoamine inhibitor, monoamine

transporter inhibitor, COMT inhibitor, MAO inhibitor and dopamine transporter inhibitor.

21. The polypharmacophore of claim 15, wherein said modifier unit is selected from the group of spacer, scaffold assembler, delivery modulator, bioactivating group, detection agent, agent to increase solubility, and targeting agent.

22. A polypharmacophore comprising the general formula **(IIA):**




**(IIA)**

wherein S comprises a scaffold unit; at least two of A, B, or C comprise a pharmacophore; one or none of A, B, or C comprise a modifier unit; and D comprises an additional modifier unit, wherein a, b, and c are each independently greater than or equal to zero, whereby the polypharmacophore interacts with at least two biological targets.

23. The polypharmacophore of claim 22, wherein said scaffold unit is synthesized using a domino reaction.

24. The polypharmacophore of claim 22, wherein said polypharmacophore is used to treat and/or prevent a condition or disease implicating biological systems which act in concert.

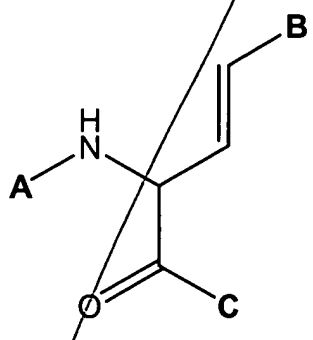
25. The polypharmacophore of claim 22, wherein said polypharmacopore is used to modulate the function of the dopaminergic system.

26. The polypharmacophore of claim 22, wherein said polypharmacophore is used to treat diseases and conditions selected from the group consisting of Alzheimer's Disease, Huntington's Disease, depression, attention deficit disorder, autism, obesity and inflammation.

27. The polypharmacophore of claim 22, wherein said pharmacophoric units are selected from the group consisting of D-1 agonist, D-2 agonist, D-3 agonist, D-4 agonist, irreversible monoamine inhibitor, reversible monoamine inhibitor, monoamine transporter inhibitor, COMT inhibitor, MAO inhibitor and dopamine transporter inhibitor.

28. The polypharmacophore of claim 22, wherein said modifier unit is selected from the group of spacer, scaffold assembler, delivery modulator, bioactivating group, and targeting agent.

29. A polypharmacophore comprising the formula **(III)**:




**(III)**

wherein at least two of A, B, or C comprise a pharmacophore; and wherein one or none of A, B, or C comprise a modifier unit, whereby the polypharmacophore interacts with at least two biological targets.

30. The polypharmacophore of claim 29, wherein said scaffold unit is synthesized using a domino reaction.

31. The polypharmacophore of claim 29, wherein said polypharmacophore is used to treat and/or prevent a condition or disease implicating biological systems which act in concert.

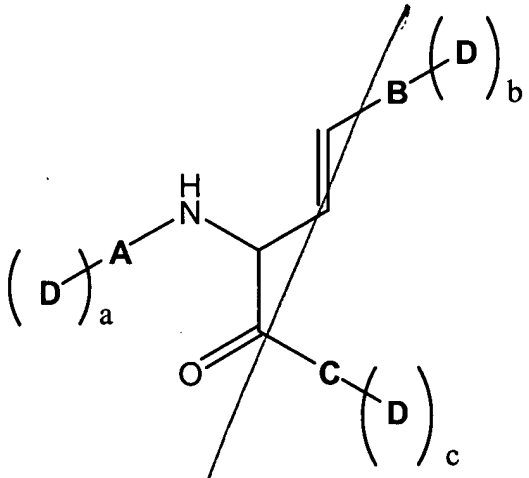
32. The polypharmacophore of claim 29, wherein said polypharmacopore is used to modulate the function of the dopaminergic system.

33. The polypharmacophore of claim 29, wherein said polypharmacophore is used to treat diseases and conditions selected from the group consisting of Alzheimer's Disease, Huntington's Disease, depression, attention deficit disorder, autism, obesity and inflammation.

34. The polypharmacophore of claim 29, wherein said pharmacophoric units are selected from the group consisting of D-1 agonist, D-2 agonist, D-3 agonist, D-4 agonist, irreversible monoamine inhibitor, reversible monoamine inhibitor, monoamine transporter inhibitor, COMT inhibitor, MAO inhibitor and dopamine transporter inhibitor.

35. The polypharmacophore of claim 29, wherein said modifier unit is selected from the group of spacer, scaffold assembler, delivery modulator, bioactivating group, detection agent, agent to increase solubility, and targeting agent.

36. A polypharmacophore comprising the formula **(IIIA):**




**(IIIA)**

wherein at least two of A, B, or C comprise a pharmacophore; one or none of A, B, or C comprise a modifier unit; and D comprises an additional modifier unit, wherein a, b, and c are each independently greater than or equal to zero, whereby the polypharmacophore interacts with at least two biological targets.

37. The polypharmacophore of claim 36, wherein said scaffold unit is synthesized using a domino reaction.

38. The polypharmacophore of claim 36, wherein said polypharmacophore is used to treat and/or prevent a condition or disease implicating biological systems acting in concert.

39. The polypharmacophore of claim 36, wherein said polypharmacopore is used to modulate the function of the dopaminergic system.

40. The polypharmacophore of claim 36, wherein said polypharmacophore is used to treat diseases and conditions selected from the group consisting of Alzheimer's Disease, Huntington's Disease, depression, attention deficit disorder, autism, obesity and inflammation.

41. The polypharmacophore of claim 36, wherein said pharmacophoric units are selected from the group consisting of D-1 agonist, D-2 agonist, D-3 agonist, D-4 agonist, irreversible monoamine inhibitor, reversible monoamine inhibitor, monoamine transporter inhibitor, COMT inhibitor, MAO inhibitor and dopamine transporter inhibitor.

42. The polypharmacophore of claim 36, wherein said modifier unit is selected from the group of spacer, scaffold assembler, delivery modulator, bioactivating group, detection agent, agent to increase solubility, and targeting agent.

43. A pharmaceutical composition comprising:

a polypharmacophore of any one of claims 1, 8, 15, 22, 29, and 36, or a pharmaceutically acceptable salt thereof; and

a pharmaceutically acceptable diluent or carrier.

44. A method for treating a disease or condition involving two or more biological sites comprising:

administering a pharmaceutically effective dose a polypharmacophore of any one of claims 1, 8, 15, 22, 29 or 26, or a pharmaceutically acceptable diluent or carrier.

45.The method of claim 44, wherein the disease or condition implicates biological systems which act in concert.

46. The method of claim 44, wherein the disease or condition implicates the dopaminergic system.

47. A library of polypharmacophores comprising any one of the polypharmacophores of claims 1, 8, 15, 22, 29, or 36.

48. The library of claim 47, wherein said library comprises at least 25 library members.

49. The library of claim 47, wherein said library comprises at least 100 library members.

50. The library of claim 47, wherein said library comprises at least 500 library members.

51. A method for determining one or more biological activities of a polypharmacophore comprising:

(a) contacting a scaffolded polypharmacophore or library of scaffolded polypharmacophores having any one of formulas **(I)**, **(IA)**, **(II)**, **(IIA)**, **(III)**, or **(IIIA)** to a biological target; and

(b) determining a statistically significant change in a biochemical activity relative to the level of biochemical activity in the absence of a scaffolded polypharmacophore.

52. A labeled compound comprising any one of the compounds of claims 1, 8, 15, 22, 29 or 36, wherein any one or more of the pharmacophoric units, scaffold units, or modifier units is labeled with a detection agent.

53. The labeled compound of claim 52, wherein said compound is labeled with a radionuclide.

54. The labeled compound of claim 53, wherein said compound is labeled with a fluorescent label.

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